

Monotonicity of the Sample Range of 3-D Data: Moments of Volumes of Random Tetrahedra

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Abstract

The sample range of uniform random points X_1, \dots, X_n chosen in a given convex set is the convex hull $\text{conv}[X_1, \dots, X_n]$. It is shown that in dimension three the expected volume of the sample range is not monotone with respect to set inclusion. This answers a question by Meckes in the negative.

The given counterexample is the three-dimensional tetrahedron together with an infinitesimal variation of it. As side result we obtain an explicit formula for all even moments of the volume of a random simplex which is the convex hull of three uniform random points in the tetrahedron and the center of one facet.

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1 INTRODUCTION

Choose random points X_1, \dots, X_n independently according to the uniform distribution in an interval $I \subset \mathbb{R}$. The convex hull $\text{conv}[X_1, \dots, X_n]$ of these random points is the well-known sample range which can also be defined as the interval $[X_{[1]}, X_{[n]}]$, where $X_{[1]} \leq \dots \leq X_{[n]}$ is the order statistic of the random points, and the endpoints $X_{[1]}, X_{[n]}$ are the extreme points of the random sample. It is trivial and immediate that the expected length of the sample range is a monotone function in I : Choosing uniform random points Y_1, \dots, Y_n in an interval $J \subset I$, one has

$$\mathbb{E}|\text{conv}[Y_1, \dots, Y_n]| \leq \mathbb{E}|\text{conv}[X_1, \dots, X_n]|, \quad (1)$$

where $|A|$ is the Lebesgue measure of the set A .

A generalization of this question to higher dimensions leads to nontrivial problems: First the definition of sample range, order statistic and extreme points is not obvious. Maybe the most natural extension of *extreme points* and *sample range* for higher dimensions is the following:

For random points $X_1, \dots, X_n \in \mathbb{R}^d$, we define the sample range to be the convex hull $\text{conv}[X_1, \dots, X_n]$, and the extreme points of the sample are those on the boundary of the sample range, i.e., the vertices of $\text{conv}[X_1, \dots, X_n]$.

The question we want to adress in this paper is the following: *Is the expected volume of the sample range a monotone function in the underlying distribution?* To make this question more precise, we assume (as the most simple example) that the points are chosen according to the uniform measure in a convex set K . Then the monotonicity question (1) reads as follows:

Assume that L, K are two d -dimensional convex sets. Choose independent uniform random points Y_1, \dots, Y_n in L and X_1, \dots, X_n in K . Is it true that $L \subset K$ implies

$$\mathbb{E}|\text{conv}[Y_1, \dots, Y_n]| \leq \mathbb{E}|\text{conv}[X_1, \dots, X_n]|? \quad (2)$$

Here, $|A|$ denotes the d -dimensional Lebesgue measure of the d -dimensional set A . The starting point for these investigations should be a check for the first nontrivial case $n = d + 1$ where the sample range is the random simplex spanned by the sample points. In this form, the question was first raised by Meckes [4] in the context of high-dimensional convex geometry.

As already mentioned, in dimension one this is immediate. It was proved by Rademacher [6] in 2012 that this is also true in dimension two. Our main result solves the three-dimensional case.

Theorem 1. *In \mathbb{R}^3 the expected volume of the sample range is in general **not** monotone in the underlying distribution. There are three-dimensional convex sets $L \subset K$ such that*

$$\mathbb{E}|\text{conv}[Y_1, \dots, Y_4]| > \mathbb{E}|\text{conv}[X_1, \dots, X_4]|, \quad (3)$$

if Y_1, \dots, Y_4 are chosen uniformly in L and X_1, \dots, X_4 in K .

That the general question (2) cannot be answered in the positive was already shown by Rademacher who, in a groundbreaking paper, gave counterexamples for dimensions $d \geq 4$ and $n = d + 1$. It remains an open problem whether there is a number N , maybe depending on K or only on the dimension of the underlying space, such that monotonicity holds for $n \geq N$. And a suitable precise formulation of the question for non-uniform measures would also be highly interesting.

For our proof, we need to construct a pair of convex sets leading to a counterexample. A serious drawback of this approach is that one is forced to compute the expected volume of a random simplex which is known to be a notorious hard problem. In dimension two, tedious but explicit computations from the nineteenth century yielded several explicit results, but starting with dimension three, the problem turns out to be out of reach in general. The only three-dimensional convex sets where the expected volume of a random simplex is known are the ball [5], the cube [10] and the tetrahedron [1]. And in higher dimensions only the ball allows for explicit results. Since numerical computations in dimension three suggest that in the neighbourhood of the cube and the ball the expected volume of a random simplex is monotone, the only potentially tractable counterexample could be the tetrahedron and a set close to it, which also is in accordance with numerical computations by Rademacher[6], and Reichenwallner and Reitzner[7].

Already the determination of the expected volume of a random simplex in a tetrahedron $T \subset \mathbb{R}^3$ was extremely hard. This question is known as Klee's problem, and after many

attempts, erroneous conjectures and numerical estimates, Reitzner and Buchta [1] proved in a long paper that for uniform random points X_1, \dots, X_4 in a tetrahedron of volume one, we have

$$\mathbb{E}|\text{conv}[X_1, \dots, X_4]| = \frac{13}{720} - \frac{\pi^2}{15\,015} = 0.01739\dots \quad (4)$$

It seems to be out of reach to compute this expectation for any other three-dimensional convex set close to T . Luckily there is a wonderful alternative approach due to Rademacher, using an infinitesimal variation of convex sets, which is stated in the following Lemma.

Lemma 1 (Rademacher [6]). *For $d \in \mathbb{N}$, monotonicity under inclusion of the map*

$$K \mapsto \mathbb{E}|\text{conv}[X_1, \dots, X_{d+1}]|,$$

where K ranges over all d -dimensional convex bodies and X_i are iid uniform points in K , holds if and only if we have for each convex body $K \subseteq \mathbb{R}^d$ and for each $z \in \text{bd } K$ that

$$\mathbb{E}|\text{conv}[X_1, \dots, X_{d+1}]| \leq \mathbb{E}|\text{conv}[X_1, \dots, X_d, z]|.$$

Hence we get the counterexample for Theorem 1 if we succeed in computing the expectation $\mathbb{E}|\text{conv}[X_1, \dots, X_3, z]|$ for some $z \in \text{bd } T$. Because of symmetry, a suitable choice for z should be the center c of one of the facets. Yet after several attempts, we observed that computing $\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|$ is even more difficult than (4) and hence impossible. Nevertheless we will prove the following proposition.

Proposition 1. *For a tetrahedron T of volume one, c the centroid of a facet of T and X_1, \dots, X_3 uniform random points in T , we have that*

$$\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]| < \frac{13}{720} - \frac{\pi^2}{15\,015} = \mathbb{E}|\text{conv}[X_1, \dots, X_4]|.$$

A combination of this result with Rademacher's Lemma 1 yields Theorem 1. The rigorous bound in Proposition 1 is obtained by combining methods from stochastic geometry with results from approximation theory. In the background, first there is a result about the precise approximation of the absolute value function on $[-\frac{1}{3}, \frac{1}{3}]$ by suitable even polynomials, Lemma 2. To apply this in our context, we use an explicit result for *all* even moments of $|\text{conv}[X_1, \dots, X_3, c]|$ which — at a first glance maybe surprisingly — is much easier to obtain than just the single first moment.

Theorem 2. *Let $k \in \mathbb{N}$ and choose three uniform random points X_1, \dots, X_3 in a tetrahedron of volume one. Then it holds:*

$$\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^{2k} = \frac{8}{3^{2k-3}} \sum_{\sum_{i=1}^{18} k_i = 2k} (-1)^{k'} 3^{k''} \binom{2k}{k_1, \dots, k_{18}} \prod_{i=1}^3 \frac{l_i! m_i! n_i!}{(l_i + m_i + n_i + 3)!},$$

where the range of summation and abbreviations are given in (7). The first five even moments are given at the end of Section 2.

This paper is organized in the following way. In Section 2, we give a series representation for even moments of the volume of a random tetrahedron inside a tetrahedron where one point is fixed to be the centroid of a facet, and we use that to find an exact value for the first thirteen even moments. In Section 3, we compute an upper bound for the expected volume of our random tetrahedron, which is a rational affine combination of those even moments. This upper bound suffices to show that the tetrahedron is a counterexample.

As a general reference for results on random polytopes, we refer to the book on Stochastic and Integral Geometry by Schneider and Weil [9]. More recent surveys are due to Hug [3] and Reitzner [8].

2 EVEN MOMENTS OF THE VOLUME OF RANDOM SIMPLICES

Let T be a tetrahedron of volume one and $c = (x_c, y_c, z_c)$ the centroid of one of its facets. For random points $X_1, X_2, X_3 \in T$, we write $X_i = (x_i, y_i, z_i)$, $i = 1, 2, 3$. The volume of the simplex with vertices X_1, X_2, X_3 and c is given by

$$|\text{conv}[X_1, \dots, X_3, c]| = \left| \frac{1}{6} \det \begin{pmatrix} x_1 & y_1 & z_1 & 1 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_c & y_c & z_c & 1 \end{pmatrix} \right| = 6^{-1} |D(x_1, \dots, z_c)|,$$

and hence by the absolute value of a polynomial D of degree precisely three in the coordinates of X_1, X_2, X_3 and c . We are interested in the even moments of $|\text{conv}[X_1, \dots, X_3, c]|$, where we get rid of the absolute value.

$$\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^{2k} = 6^{-2k} \int_T \int_T \int_T D(x_1, \dots, z_c)^{2k} d(x_1, y_1, z_1) d(x_2, y_2, z_2) d(x_3, y_3, z_3).$$

Let T_o be the specific tetrahedron

$$T_o = \{(x, y, z) \in \mathbb{R}^3 : x, y, z \geq 0, x + y + z \leq 1\},$$

i.e., that with vertices $(0, 0, 0)$, $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$. Note that the volume of T_o is $1/6$. We choose $c_o = (1/3, 1/3, 0)$, the centroid of the facet $\{(x, y, 0) \in \mathbb{R}^3 : x, y \geq 0, x + y \leq 1\}$.

Since the expectation $\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|$ is invariant under volume-preserving affine transformations, we can use as a representative of a tetrahedron of volume one the tetra-

hedron $\sqrt[3]{6} T_o$ and the center $\sqrt[3]{6} c_o$. We have:

$$\begin{aligned}
 \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^{2k} &= 6^{-2k} \int_{\sqrt[3]{6} T_o} \int_{\sqrt[3]{6} T_o} \int_{\sqrt[3]{6} T_o} D(x_1, \dots, z_{\sqrt[3]{6} c_o})^{2k} \\
 &\quad d(x_1, y_1, z_1) d(x_2, y_2, z_2) d(x_3, y_3, z_3) \\
 &= 6^3 \int_{T_o} \int_{T_o} \int_{T_o} D(x_1, \dots, z_{c_o})^{2k} d(x_1, y_1, z_1) d(x_2, y_2, z_2) d(x_3, y_3, z_3). \quad (5)
 \end{aligned}$$

Expanding the determinant, the polynomial D can be written as

$$\begin{aligned}
 D(x_1, \dots, z_{c_o}) = \frac{1}{3} &\left(x_1 z_2 - x_1 z_3 - x_2 z_1 + x_2 z_3 + x_3 z_1 - x_3 z_2 - y_1 z_2 + y_1 z_3 \right. \\
 &\quad + y_2 z_1 - y_2 z_3 - y_3 z_1 + y_3 z_2 + 3x_1 y_2 z_3 - 3x_1 y_3 z_2 \\
 &\quad \left. - 3x_2 y_1 z_3 + 3x_2 y_3 z_1 + 3x_3 y_1 z_2 - 3x_3 y_2 z_1 \right).
 \end{aligned}$$

By the Multinomial Theorem, and using the multinomial coefficient

$$\binom{2k}{k_1, \dots, k_{18}} = \frac{(2k)!}{k_1! \cdots k_{18}!},$$

the $(2k)$ -th power of it can be rewritten as

$$\begin{aligned}
 D(x_1, \dots, z_{c_o})^{2k} &= 3^{-2k} \sum_{\sum_1^{18} k_i = 2k} (-1)^{k'} 3^{k''} \binom{2k}{k_1, \dots, k_{18}} (x_1 z_2)^{k_1} (x_1 z_3)^{k_2} (x_2 z_1)^{k_3} \\
 &\quad \times (x_2 z_3)^{k_4} (x_3 z_1)^{k_5} (x_3 z_2)^{k_6} (y_1 z_2)^{k_7} (y_1 z_3)^{k_8} (y_2 z_1)^{k_9} \\
 &\quad \times (y_2 z_3)^{k_{10}} (y_3 z_1)^{k_{11}} (y_3 z_2)^{k_{12}} (x_1 y_2 z_3)^{k_{13}} (x_1 y_3 z_2)^{k_{14}} \\
 &\quad \times (x_2 y_1 z_3)^{k_{15}} (x_2 y_3 z_1)^{k_{16}} (x_3 y_1 z_2)^{k_{17}} (x_3 y_2 z_1)^{k_{18}} \\
 &= 3^{-2k} \sum_{\sum_1^{18} k_i = 2k} (-1)^{k'} 3^{k''} \binom{2k}{k_1, \dots, k_{18}} \prod_{i=1}^3 x_i^{l_i} y_i^{m_i} z_i^{n_i}. \quad (6)
 \end{aligned}$$

Here for abbreviation we use the following notation:

$$\begin{aligned}
k' &= k_2 + k_3 + k_6 + k_7 + k_{10} + k_{11} + k_{14} + k_{15} + k_{18}, \\
k'' &= k_{13} + k_{14} + k_{15} + k_{16} + k_{17} + k_{18}, \\
l_1 &= k_1 + k_2 + k_{13} + k_{14}, \\
m_1 &= k_7 + k_8 + k_{15} + k_{17}, \\
n_1 &= k_3 + k_5 + k_9 + k_{11} + k_{16} + k_{18}, \\
l_2 &= k_3 + k_4 + k_{15} + k_{16}, \\
m_2 &= k_9 + k_{10} + k_{13} + k_{18}, \\
n_2 &= k_1 + k_6 + k_7 + k_{12} + k_{14} + k_{17}, \\
l_3 &= k_5 + k_6 + k_{17} + k_{18}, \\
m_3 &= k_{11} + k_{12} + k_{14} + k_{16}, \\
n_3 &= k_2 + k_4 + k_8 + k_{10} + k_{13} + k_{15}.
\end{aligned} \tag{7}$$

Integration of the monomials over the tetrahedron T_o gives

$$\begin{aligned}
\int_{T_o} x^{l_i} y^{m_i} z^{n_i} d(x, y, z) &= \underbrace{\int_0^1 \int_0^1 \int_0^1}_{x+y+z \leq 1} x^{l_i} y^{m_i} z^{n_i} dx dy dz \\
\left| \begin{array}{l} z = t \\ y = s(1-t) \\ x = r(1-s)(1-t) \end{array} \right| &= \int_0^1 r^{l_i} dr \int_0^1 s^{m_i} (1-s)^{l_i+1} ds \int_0^1 t^{n_i} (1-t)^{l_i+m_i+2} dt \\
&= \frac{1}{l_i+1} B(m_i+1, l_i+2) B(n_i+1, l_i+m_i+3) \\
&= \frac{l_i! m_i! n_i!}{(l_i+m_i+n_i+3)!}.
\end{aligned}$$

Combining this with equations (5) and (6) yields

$$\begin{aligned}
\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^{2k} &= \\
&= \frac{8}{3^{2k-3}} \sum_{\sum_1^{18} k_i = 2k} (-1)^{k'} 3^{k''} \binom{2k}{k_1, \dots, k_{18}} \prod_{i=1}^3 \frac{l_i! m_i! n_i!}{(l_i+m_i+n_i+3)!},
\end{aligned}$$

which is Theorem 2. We list the first five even moments of the volume of a random simplex

in a tetrahedron T of volume one:

$$\begin{aligned}\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^2 &= \frac{1}{2000} = 0.0005, \\ \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^4 &= \frac{43}{27\,783\,000} \approx 1.54771 \cdot 10^{-6}, \\ \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^6 &= \frac{347}{28\,805\,414\,400} \approx 1.20463 \cdot 10^{-8}, \\ \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^8 &= \frac{2\,389}{14\,263\,395\,300\,000} \approx 1.67492 \cdot 10^{-10}, \\ \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^{10} &= \frac{310483}{90\,249\,636\,885\,408\,000} \approx 3.44027 \cdot 10^{-12}.\end{aligned}$$

3 PROOF OF THEOREM 1

As described in Section 2, the $(2k)$ -th moment of $|\text{conv}[X_1, \dots, X_3, c]|$ can be computed, with fast increasing complexity in k . Also note that the volume of a tetrahedron in T , where one vertex is fixed to be the centroid of a facet of T , is not larger than $1/3$. Hence, we want to approximate the absolute value function in the interval $[-1/3, 1/3]$ by a polynomial

$$P(x) = \sum_{i=0}^n a_i x^{2i}$$

for some $n \in \mathbb{N}$ such that $P(x) > |x|$ for all $x \in [-1/3, 1/3]$ or, equivalently, $P(x) > x$ for all $x \in [0, 1/3]$. In contrast to the classical problem of *best approximation* of $|x|$ by polynomials, we are interested in one-sided approximation and a certain expected value of the polynomial as objective. We use the following standard result for polynomial interpolation.

Lemma 2. *Let $m \in \mathbb{N}$, $n = 2m + 1$, and $0 < x_0 < \dots < x_m$ be given. Then the system of equations*

$$P(x_j) = x_j \text{ and } P'(x_j) = 1 \quad \text{for } j = 0, \dots, m$$

determines uniquely a polynomial $P(x) = \sum_{i=0}^n a_i x^{2i}$ with the property $P(x) \geq |x|$ for all $x \in \mathbb{R}$.

Proof. Let $t_j = x_j^2$ and consider the standard Hermite interpolation problem

$$Q(t_j) = f(t_j) \text{ and } Q'(t_j) = f'(t_j) \quad \text{for } j = 0, \dots, m$$

for the functions $f(t) = \sqrt{t}$ and $Q(t) = \sum_{i=0}^n a_i t^i$. The condition $P'(x_j) = 1$ is equivalent to $Q'(t_j) = 1/(2\sqrt{t_j}) = f'(t_j)$. Then the interpolation error fulfills, for some $\xi \in [t_0, t_m]$, the estimate

$$f(t) - Q(t) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{j=0}^m (t - t_j)^2 < 0,$$

where the last inequality follows from $f^{(n+1)}(t) < 0$ for all t . □

We note in passing that for even $n = 2m$ and $0 < x_0 < \dots < x_m = 1/3$, we only require the simple interpolation condition $P(x_m) = x_m$ in the last point and get $P(x) \geq |x|$ for all $x \in [-x_m, x_m]$.

Our aim is to approximate $\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|$ from above by an even polynomial P of degree $2n$,

$$\mathbb{E}|\text{conv}[X_1, \dots, X_3, c]| \leq \mathbb{E}P(|\text{conv}[X_1, \dots, X_3, c]|),$$

which holds if $|x| \leq P(x)$ on $[-\frac{1}{3}, \frac{1}{3}]$. Moreover, the best polynomial for fixed $n \in \mathbb{N}$ can be found via the linear optimization problem

$$\begin{aligned} \min_P \mathbb{E}P(|\text{conv}[X_1, \dots, X_3, c]|) &= \min_{a_i} \sum_{i=0}^n a_i \mathbb{E}P(|\text{conv}[X_1, \dots, X_3, c]|)^{2i} \\ \text{s.t. } P(x) &\geq x, \quad x \in \left[0, \frac{1}{3}\right]. \end{aligned}$$

Please note that the constraint is infinite dimensional. Relaxing the constraint, we get a lower bound on $\mathbb{E}P(|\text{conv}[X_1, \dots, X_3, c]|)$ via the finite dimensional linear program

$$\min_P \mathbb{E}P(|\text{conv}[X_1, \dots, X_3, c]|) \quad \text{s.t. } P(x_\ell) \geq x_\ell, \quad x_\ell \in \left[0, \frac{1}{3}\right], \quad \ell = 0, \dots, L.$$

For $n = 12$ and $L = 100$ equidistant points $x_\ell \in [0, 1/3]$, we numerically compute via Matlab and the optimization toolbox CVX [2]

$$\mathbb{E}P(|\text{conv}[X_1, \dots, X_3, c]|) > 0.01746,$$

yielding that we do not get a sufficiently precise estimate using only $n = 12$ even moments.

For $n = 13$ and $L = 1000$, we solved the above linear program, computed the interpolation nodes with the absolute value function numerically, and rationalized these points to

$$\{x_j : j = 0, \dots, 6 = m\} = \left\{ \frac{1}{83}, \frac{1}{22}, \frac{1}{11}, \frac{2}{15}, \frac{2}{11}, \frac{5}{22}, \frac{4}{15} \right\}.$$

Using these points for the interpolation problem in Lemma 2 gives an even polynomial $P_{\text{cert}}(x) = \sum_{i=0}^{13} a_i x^{2i}$ of degree 26 with explicitly given rational coefficients a_0, \dots, a_{13} and the property $|x| \leq P_{\text{cert}}(x)$. Finally, we use the even moments computed in Section 2 to complete the proof of Theorem 1:

$$\begin{aligned} \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]| &\leq \mathbb{E}P_{\text{cert}}(|\text{conv}[X_1, \dots, X_3, c]|) = \sum_{i=0}^{13} a_i \mathbb{E}|\text{conv}[X_1, \dots, X_3, c]|^{2i} \\ &= \underbrace{\frac{9215716290354841120429638007455369524673678722793816500930077456473045568887048115406728916177539584718665872679760706490830685597508152285959465854826727651}{5302749610595656531552835250244971867247891347471652937573234276503331818475900122041632848466907674944123592136803582459020919668764372661702456688640000000000}}_{=0.0173791\dots} \\ &< \underbrace{\frac{13}{720} - \frac{\pi^2}{15015}}_{=0.01739\dots} = \mathbb{E}|\text{conv}[X_1, \dots, X_4]|. \end{aligned}$$

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